

# Cooling of a small sample of Bose atoms with accidental degeneracy

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A system of bosons in a harmonic trap is cooled via their interactions with a thermal reservoir. We derive the master equation that governs the evolution of the system and may describe diverse physical situations: laser cooling, sympathetic cooling, etc. We investigate in detail the dynamics of the gas in the Lamb-Dicke limit, whereby the size of the trap is small in comparison to the de Broglie wavelength of the reservoir quanta. In this case, the dynamics is characterized by two time scales. First, an equilibrium is reached on a *fast time scale* within the degenerated subspaces of the system. Then, an equilibrium between these subspaces is reached on a *slow time scale*.

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## I. INTRODUCTION

### A. Bose-Einstein condensation

The observation of effects related to the quantum statistical properties of weakly interacting gases of atoms [1] has become in the last decades a major challenge of atomic physics. Thus, a large part of the theoretical and experimental research has been focused during the 90's on cooling atoms confined in traps at relatively high densities [2]. These studies have led to the remarkable experimental realisation of a Bose-Einstein condensation (BEC) in Rubidium [3], and sodium vapors [4]. Evidence of BEC in a Lithium gas with attractive interactions has been also reported [5]. These remarkable achievements, have opened fascinating possibilities and applications, such as the development of a coherent source of atoms, or *atom laser* [6].

The theoretical description of a system of ultracold bosonic or fermionic atoms is particularly convenient in the framework of second quantization. Quantum field theories of cold atoms [7], originally developed in a condensed-matter context, have been used in the diagnostics of a Bose-Einstein condensate [8], and in *nonlinear atomic optics* [9].

Several theoretical works in the recent years were more directly aimed to the dynamics of the cooling processes, dynamics of the possible phase transitions and the formation of quantum collective states. Those works concern both *collisional cooling* mechanisms, such as evaporation [10,11] or sympathetic cooling [12–15], or *laser cooling* mechanisms, such as sideband cooling [16], Raman cooling [17], and dark state cooling [18]. The latter processes allow to reach temperatures below the photon recoil energy  $E_R$  [equal to  $(\hbar k)^2/(2M)$ , where  $k$  is the laser wavevector and  $M$  the atomic mass]. One expects that the system might then enter a collective quantum state (such as Bose-Einstein condensate, or some analogue of it). In particular, under such conditions one hopes to realize also a coherent source of atoms.

### B. Quantum Master Equation

In general, the quantum dynamics of a system of cold atoms is a very complex many-body problem. Some of the above mentioned processes may be analyzed using quantum Boltzmann equations [19,20]. Starting from 1994 a more general method based on a quantum master equation (QME) description [21] has been developed. In particular, a QME describing the dynamics of a small sample of laser cooled atoms in a harmonic microtrap has been proposed and analyzed [22]. The quantum statistical nature of the atoms is reflected in the dynamics of the cooling process. In the case when the trapping potentials for the atoms in the ground and excited electronic states are different such QME might lead to multistability and *generalized Bose-Einstein distributions* [23]. The QME has the advantage that it permits to study atom number fluctuations in each of the trap levels, and thus provides a more complete description of the cooling process. In particular, it may be used, in principle, to describe the dynamics of condensate formation. We have also derived a QME for sympathetic cooling [24] and analyzed the possibility of achieving the condensation of a system of light particles which interact with a reservoir of heavier particles. In the context of nonlinear atomic optics a self-consistent Born-Markov-Hartree-Fock master equation has been derived and analyzed to study the spontaneous emission effects on atomic solitons [25].

Since that early works, the theory of QME for many-body systems has been very strongly developed. In particular, C. Gardiner, P. Zoller and co-workers developed in a series of papers [26] the QME and Quantum Kinetic Boltzmann approach to describe the dynamics of the evaporative cooling. We have also extended the theory of the collective laser cooling to much more realistic situations, avoiding the microtrap assumption, and working beyond the so-called Lamb-Dicke limit, in which the trap is of the size of the laser wavelength [27]. In such

analysis, we avoided the reabsorption problem by working in the so-called *Festina Lente* regime, in which the spontaneous emission rate is smaller than the trap frequency.

One should stress that, apart from the area of quantum optics, master equations for quantum Bose or Fermi gases have been used in statistical physics [28]. However, the master equation is usually postulated there starting from general statistical requirements. It describes the approach towards the thermal equilibrium described by the Bose-Einstein or, correspondingly, Fermi-Dirac distributions, it fulfills detailed balance conditions, and sometimes it conserves some order parameters. The dynamics that it generates might have some universal properties, but does not have a direct physical interpretation in terms of interaction with specific energy reservoirs.

In most of the quantum optical examples, the master equation is derived via the elimination of the “bath” degrees of freedom starting from a more general theory that describes a very specific physical situation. The eliminated “bath” has a direct physical interpretation - it consists of photons, colliding atoms etc. Each of the jumps between the states of the system described by the QME usually corresponds to a very well defined physical process of photon emission, absorption, atom-atom collision etc. [29].

The QME approach, although valid in general, can only be used for practical calculations when the QME can be reduced to a set of kinetic equations, while the density matrix to a diagonal form. Such reduction is not always possible, and very often requires first the choice of an appropriate basis in the Hilbert space of the states of the system. In particular, the *bare* states of the system, that are the eigenstates of the system Hamiltonian in isolation from the “bath”, are not necessarily the right ones. For instance, in the process of cooling of an ideal bosonic gas confined in a microtrap, the reduction in the basis of *bare* states is possible only if additional assumptions are made. These statements seem a little surprising, since they hold even for arbitrary weak system-“bath” interactions, i.e. a situation in which the quantum Boltzmann equations should be valid [20]. Note, however, that the validity of the quantum Boltzmann equations usually requires assumptions concerning quantum ergodicity, which simply do not hold in the above mentioned situations. The point here is that an ideal bosonic gas in a harmonic trap has plenty of degenerated *bare* energy levels. The quantum coherences between those levels (i.e. non-diagonal elements of the density matrix) can survive for very long times, and contribute significantly to the dynamics.

### C. Degeneracy in many-body systems

Let us enumerate by  $\vec{m}$  the eigenstates of a *single atom* Hamiltonian in the rotationally symmetric harmonic trap of frequency  $\omega$ , where  $\vec{m}$  is a natural number in one di-

mension, a pair of natural numbers in 2D, a triple in 3D etc. When we consider an ensemble of  $N$  atoms, the states of such an *ideal gas* can be written in the Fock representation as  $|n_{\vec{0}}, n_{\vec{1}}, \dots\rangle$ , where  $n_{\vec{m}}$  denote the occupation numbers of the corresponding  $\vec{m}$ -th eigenstate. For noninteracting atoms there are two kinds of degeneracies in such a system. First, a degeneracy of energy levels due to rotational invariance; that is for the states for which the sum of  $n_{\vec{m}}$ ’s with a fixed sum of the components of  $\vec{m}$ , is fixed itself. Obviously, such degeneracies are not present in 1D. We shall not discuss them here. Second, there exists an *accidental* degeneracy, due to the particular symmetry of the harmonic potential [30]. This degeneracy occurs even in the case of 1D: for instance for the states  $|0, 2, 0, \dots\rangle$  and  $|1, 0, 1, 0, \dots\rangle$ . Here, the state with two atoms in the first energy level has an energy  $2 \times \hbar\omega$ , which is equal to the energy of the state with one atom in the ground level and another atom in the second excited level ( $1 \times 0\hbar\omega + 1 \times 2\hbar\omega$ ). Both kinds of degeneracies are lifted up if one considers anisotropic trap with anharmonic energy levels. If one then assumes that the resulting energy level shifts are larger than cooling rates, one can evoke standard secular arguments to reduce the master equation to a diagonal form in the basis of the *bare* ideal gas states [22]. It is precisely the subject of the present paper to study the situation in which such reduction is not possible, i.e. when the effects of accidental degeneracy dominate the dynamics of the system.

One could argue that such problem is purely academic since in real physical system atom-atom interaction will always lift the accidental degeneracy. The whole point is, however, that as long as the interactions are not too strong, the system will still exhibit effects of *quasi-degeneracy*. This will be the case when energy differences between the quasi-degenerated levels will be small in comparison to  $\hbar\omega$ . Such condition is realised in not too dense systems, i.e. the system containing not too many atoms. The idealized theory presented in this paper is formulated for arbitrary number of atoms  $N$ , but in practice it applies to the situation when  $N$  is not too large (see Section VII). Nevertheless, in view of the complexity of the problem, it is in our opinion reasonable to treat the ideal case of non-interacting atoms in order to get insight into more realistic cases. That said, let us note at this point that in the last years the external modification of the s-wave scattering length (which dominates the atom-atom collisions at low energies), has been theoretically investigated in different scenarios [31], and also experimentally demonstrated by employing the so-called Feshbach resonances [32,33]. Remarkably, very recent experimental results show that a modification of the scattering length to very small values is experimentally feasible [33], opening the fascinating possibility to achieve a quasi-ideal bosonic gas, as that studied in the present paper.

## D. Content of the paper

The paper concerns thus the problem of cooling of an *ideal* Bose gas, or more precisely speaking a sample consisting of  $N$  atoms, in a *perfectly harmonic microtrap*. It should be noted that this problem is quite general. Atomic traps, although frequently anisotropic (see for example Ref. [3]), can be designed to be, with a very good accuracy, harmonic. Moreover, even though in the small atomic samples atom-atom interactions will lift the exact degeneracy of energy levels, the system will remain *quasi-degenerated*. We expect that a cooled atomic sample in such a harmonic microtrap will exhibit the effects of accidental quasi-degeneracy *regardless of the method used for its cooling*. In order to stress this general aspect of our study, we adopt here partially the statistical physics approach, and derive a master equation using a phenomenological model of the “bath”. In particular, our “bath” may represent one of the following two reservoirs: B1) a photon reservoir in the case of laser cooling [22]; B2) an atomic reservoir consisting of other atoms in the case of symphatetic cooling [24]. In the case B2) the bath atoms are trapped in a larger trap than the system atoms. Such situation (proposed and discussed in [24]) could be realised if a small, say far-off-resonance dipole trap for system atoms was located inside a larger magnetic trap for the bath atoms [34].

Given that the resulting master equations for all these reservoirs have the same structure, the qualitative behavior for the cooling dynamics given by our specific model is quite general. The reason why we have chosen such a model for the bath is that it has the advantage that one can derive analytical formulas for the transition rates between different levels. We also stress that the mathematical treatment developed in this paper can be easily generalized to other physical situations, in particular for ultra-cold trapped polarised Fermi gases, which due to the suppression of the  $s$ -wave scattering induced by the Pauli principle, can be in an excellent approximation as ideal gases [35].

This paper is organized as follows: In Section II we introduce the model, describing separately the system in a trap, the atomic bath, and the system-bath interactions. This Section is very much analogous to Section II of Ref. [24], but is formulated for a different model of the bath. In Section III we derive the master equation governing the dynamics of the system, under Born and Markov approximations. This equation is further analyzed in Section IV in the microtrap limit in terms of the Lamb-Dicke (LD) expansion, i.e. a systematic expansion in a small parameter  $\eta = ka$ , where  $a$  is the size of the trap ground state wavefunction, whereas  $k$  is a typical wavevector of the bath quanta that is relevant for the cooling process. In Section V we discuss explicitly the breakdown of ergodicity due to the accidental degeneracy that occurs on a fast time scale in the lowest order of the LD expansion. Section VI is devoted to the discussion of the restoration

of ergodicity on a slower time scale due to higher orders of LD expansion, whereas Section VII contains our conclusions. The paper also contains three appendices. Appendix A contains some useful formulas of the operator algebra used in the paper, and describes the structure of the Hilbert space. Appendix B describes the details of the construction of some of the multiple vacua that appear due to the accidental degeneracy, whereas Appendix C presents matrix elements of the second quantized operators used in the paper. These elements are used for some calculations regarding the cooling rates. Finally, in Appendix D we present a proof of the decay of coherences on the slow time scale.

## II. DESCRIPTION OF THE MODEL

We consider a system “A” of bosonic particles that are confined in a trap, and interact with a bath bosonic particles “B”. We assume that the particles “B” are practically not affected by their interactions with the system “A”, so that “B” can be regarded as a phenomenological reservoir for “A”. The coupling to the bath represents the influence of some externally controlled cooling mechanism (laser cooling, symphatetic cooling, etc.) on the system “A”. The reservoir is assumed to be in thermal equilibrium at some given temperature. In this Section we introduce the Hamiltonian for the system “A”, the bath “B”, and for their mutual interactions. The formalism is developed for the case of  $d$  spatial dimensions.

### A. Description of the system

The system “A” is an *ideal gas* of  $N$  bosonic atoms of mass  $M_A$  confined by an isotropic harmonic potential in  $d$  dimensions. In a second quantized form, and in the Fock representation the Hamiltonian describing the system can be written in the form

$$H_A = \sum_{\vec{n}} \hbar\omega(n_x + n_y + \dots) a_{\vec{n}}^\dagger a_{\vec{n}}, \quad (1)$$

where  $\omega$  is the trap frequency,  $\vec{n} = (n_x, n_y, \dots)$  with  $n_x, n_y, \dots = 0, 1, 2, \dots$ , and  $a_{\vec{n}}^\dagger$  and  $a_{\vec{n}}$  are creation and annihilation operators of particles in the  $\vec{n}$ -th level of the harmonic potential, respectively. Since in the present paper we are interested in the effects of the accidental degeneracy, we neglect the contribution of the atom-atom interactions to the total Hamiltonian (for the discussion of its role see [22–24], and Section VII).

### B. Bath

Similarly as in Ref. [24], we assume that the system “B” contains a practically infinite number of bosons of mass  $M_B$  embedded in a practically infinite volume, with

finite density  $n_B$ . The free Hamiltonian for the bath “B” of particles in a second quantized form is

$$H_B = \int d\vec{k} \epsilon(\vec{k}) b(\vec{k})^\dagger b(\vec{k}). \quad (2)$$

Here,  $\vec{k}$  is a wavevector in a  $d$ -dimensional space. The function  $\epsilon(\vec{k})$  represents the dispersion relation of the bath particles. For instance, for quasi-free particles it reads

$$\epsilon(\vec{k}) = \frac{(\hbar k)^2}{2M_B}, \quad (3)$$

where  $M_B$  is the *effective mass* of the bath “quanta”. In the following we shall use Eq. (3) but the theory is easily generalized to arbitrary shapes of the dispersion relation. In particular, we shall also consider massless bath quanta with a photonic-like linear dispersion relation. Note that such dispersion relation is in fact appropriate for both types of bath (B1), and (B2) mentioned above. This is obvious in the case of laser cooling, but is also true for collisional cooling schemes, since no mass is produced or lost in the collision processes. The operators  $b(\vec{k})^\dagger$  and  $b(\vec{k})$  are creation and annihilation operators of bath particles corresponding to plane wave states with momentum  $\vec{k}$ . In the case of laser cooling (B1)  $\vec{k}$  corresponds to a photon momentum, whereas in the case (B2)  $\vec{k}$  is rather a *momentum transfer* associated with the system atom-bath atom collision. The operators  $b(\vec{k})^\dagger$  and  $b(\vec{k})$  fulfill the usual commutation relations

$$\begin{aligned} [b(\vec{k}), b(\vec{k}')] &= [b(\vec{k})^\dagger, b(\vec{k}')^\dagger] = 0, \\ [b(\vec{k}), b(\vec{k}')^\dagger] &= \delta^{(d)}(\vec{k} - \vec{k}'). \end{aligned}$$

In thermal equilibrium, the density operator describing the state of the bath  $\rho_B$  corresponds to the usual Bose–Einstein distribution (BED) [36]. In this situation, we have

$$\langle b(\vec{k}) b(\vec{k}') \rangle = \langle b(\vec{k})^\dagger b(\vec{k}')^\dagger \rangle = 0, \quad (4a)$$

$$\langle b(\vec{k})^\dagger b(\vec{k}') \rangle = n(\vec{k}) \delta^{(d)}(\vec{k} - \vec{k}'), \quad (4b)$$

where  $n(\vec{k})$  is related to the number of particles with wavevector  $\vec{k}$ , and is given by

$$n(\vec{k}) = \frac{ze^{-\beta\epsilon(\vec{k})}}{1 - ze^{-\beta\epsilon(\vec{k})}}. \quad (5)$$

In the above expression,  $\beta = 1/(k_B T)$  is the inverse temperature, and  $z = \exp(\beta\mu)$  is the fugacity, while  $\mu$  denotes the chemical potential. Note that  $\mu = 0$ ,  $z = 1$  for massless quanta, and for massive particles below the condensation point. Note also that both  $n(\vec{k})$  and  $\epsilon(\vec{k})$  only depend on  $k \equiv |\vec{k}|$ . Particle and energy densities are connected with these quantities by the relations

$$n_B = \frac{1}{(2\pi)^d} \int d\vec{k} n(\vec{k}), \quad (6a)$$

$$\epsilon_B = \frac{1}{(2\pi)^d} \int d\vec{k} n(\vec{k}) \epsilon(\vec{k}), \quad (6b)$$

respectively.

### C. Interactions

Within the present model the interactions between the particles and the bath describe the annihilation of an atom followed by its immediate recreation, accompanied by absorption or emission of a single bath quantum. We have chosen such a model for the interactions since it is the simplest one that retains the effect produced by the accidental degeneracy in the cooling process. In any case, it may be regarded as a phenomenological interaction that may be due to various physical mechanisms (system atom-bath atom collisions, laser-atom interactions, etc.). Similarly to the case of atom-atom collisions we employ here an analogue of the *shape-independent approximation* [37,38] to write down the corresponding atom-bath quantum interactions. We assume that these interactions are local (i.e. have a zero range) in the spatial representation. Mathematically, this approximation means that the wave functions of both kinds of particles do not change significantly over distances characterizing interparticle potential in the relevant energy range. In the Fock representation the interaction Hamiltonian is given by

$$H_{A-B} = \sum_{\vec{n}, \vec{n}'} \int d\vec{x} \gamma_{\vec{n}, \vec{n}'}(\vec{x}) a_{\vec{n}}^\dagger a_{\vec{n}'} b^\dagger(\vec{k}), \quad (7)$$

where

$$\gamma_{\vec{n}, \vec{n}'}(\vec{k}) = \frac{\kappa}{(2\pi)^d} \int d\vec{x} \psi_{\vec{n}}(\vec{x})^* \psi_{\vec{n}'}(\vec{x}) e^{-i\vec{k}\vec{x}}, \quad (8)$$

$\psi_{\vec{n}}(\vec{x})$  is the wavefunction corresponding to the  $\vec{n}$ -th level of the harmonic oscillator, and  $\kappa$  is a coupling constant. We have chosen the form of the interaction Hamiltonian (7), because of its simplicity. We stress, however, that the qualitative (and to some extend quantitative) results of the paper do not depend on the particular choice of  $H_{A-B}$ .

Without loss of generality, we can exclude from the integration over  $\vec{k}$  in (7) the value  $\vec{k} = 0$ . This is clear since

$$\begin{aligned} \sum_{\vec{n}, \vec{n}'} \gamma_{\vec{n}, \vec{n}'}(0) a_{\vec{n}}^\dagger a_{\vec{n}'} b^\dagger(0) &\propto \\ &\left( \sum_{\vec{n}} a_{\vec{n}}^\dagger a_{\vec{n}} \right) (b^\dagger(0)), \end{aligned} \quad (9)$$

is a constant shift operator of the zero momentum mode, proportional to the number of particles in the system

“A”. One can always perform a unitary shift transformation of  $b(0)$ , and  $b^\dagger(0)$  that cancels the term (9) and its hermitian conjugate in the Hamiltonian. Obviously, such transformation modifies the BED for the bath quanta with zero momentum, but the latter modification has no relevance for the transformed system-bath interactions in which the coupling to the bath zero mode is absent. Hence, from now on, in the integrals over  $\vec{k}$  it will be implicitly assumed that  $\vec{k} \neq 0$ . On the other hand, since in the next Section we are going to make a rotating wave approximation (RWA) in the master equation derived from the Hamiltonian (7), we reduce Eq. (7) (as in Ref. [24]) to the form

$$H_{A-B} = H_0 + \sum_{\alpha=1}^{\infty} (H_{\alpha} + H_{\alpha}^{\dagger}). \quad (10)$$

Here,  $H_0$  contains the part of  $H_{A-B}$  given in (7) in which the sum is extended over values with  $\sum_{s=x,y,\dots} (n_s - n'_s) = 0$ .  $H_{\alpha}$  contains the part of  $H_{A-B}$  proportional to the bath annihilation operators  $b(\vec{k})$ , with the sum over  $\vec{n}, \vec{n}'$  extended over the values for which  $\sum_{s=x,y,\dots} (n_s - n'_s) = \alpha$ .

The QME that we shall derive in the next Section will contain a Hamiltonian part (describing energy level shifts), and non-Hamiltonian part describing dissipative decay processes. It is worth mentioning that due to the RWA the Hamiltonian part of the master equation will not be generally correct [21,39]. However, as in Ref. [24], we will be only interested in the dissipative part of the master equation, which is correctly described under the mentioned RWA, provided the trap frequency  $\omega$  is larger than the cooling rates. The latter assumption will be made all over the present paper.

### III. DERIVATION OF THE MASTER EQUATION

The master equation for the above defined model can be derived following well-established procedures in the field of quantum optics [21,39], analogously to those discussed in Ref. [24]. We first move to an interaction picture defined by the unitary operator  $\exp[-i(H_A + H_B)t]$ . In this picture, the density operator  $\tilde{\rho}$  describing system-plus-bath degrees of freedom fulfills the following equation:

$$\frac{d\tilde{\rho}(t)}{dt} = -\frac{i}{\hbar} [\tilde{H}_{A-B}(t), \tilde{\rho}(t)], \quad (11)$$

where the tilde indicates that the operators are expressed in the interaction picture. We integrate formally this equation, and substitute back into (11). Next, we define the reduced density operator for system “A”,  $\rho_A = \text{Tr}_B(\rho)$ , where  $\text{Tr}_B$  stands for the trace over the bath states, and make use of the fact that  $\text{Tr}_B\{[H_{A-B}(0), \rho(0)]\} = 0$ , since we assume that the density operator for the bath  $\rho_B(0)$  is diagonal in the

Fock basis (with respect to  $H_B$ ), whereas  $H_{A-B}$  does not contain any diagonal matrix elements [the reader should recall that we have extracted the terms with  $\vec{k} = 0$  in  $H_{A-B}$ , see Eq. (7)]. We obtain the following equation:

$$\frac{d\tilde{\rho}_A(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t d\tau \text{Tr}_B\{[\tilde{H}_{A-B}(t), [\tilde{H}_{A-B}(t-\tau), \tilde{\rho}(t-\tau)]]\}. \quad (12)$$

In the following step we perform Born–Markov approximation. For this approximation we have to assume that the correlation time  $\tau_c$  of the reservoir is much shorter than the typical time over which  $\tilde{\rho}_A(t)$  changes, i.e. the cooling time [39]. The Born–Markov approximation is also related to the fact that the bath quanta are practically not affected by their interactions with the system; this allows us to write  $\tilde{\rho}(t-\tau) = \tilde{\rho}_A(t-\tau) \otimes \rho_B(0)$ . From the technical point of view, the correlation time  $\tau_c$  can be defined as a time for which the integrand of (12) practically vanishes. For specific physical models of the bath it can be directly evaluated (see, for instance, Ref. [24]). The cooling time, on the other hand, depends on the physics of the interactions between atoms and bath quanta. It is *controllable*, and thus is assumed to be the longest time scale of the problem. In this case, we can safely substitute  $\tilde{\rho}_A(t-\tau)$  by  $\tilde{\rho}_A(t)$  in the integral (12), and extend the upper limit of the integral to infinity.

In the next steps we make use of Eq. (10) and perform the RWA, i.e. neglect terms rotating at multiples of the trap frequency. Again, this approximation is based on the assumption that trap frequencies are large in comparison to the cooling rates.

Finally, taking into account the bath properties (4), and coming back to the Schrödinger picture we obtain the following master equation:

$$\frac{d\rho_A}{dt} = -\frac{i}{\hbar} [H_A + H'_{A-A}, \rho_A] + \mathcal{L}\rho_A, \quad (13)$$

where  $H'_{A-A}$  is the Hamiltonian term produced by the elimination of the bath in the master equation. Physically, this term accounts for the energy level shifts due to the effective interaction between system particles via their interactions with the bath quanta.  $H'_{A-A}$  may also include the original atom-atom interactions (provided they were present in the original Hamiltonian) in the spirit of *independent rates approximation* [39]. Similarly as in the case of the atom-atom collisions, all of the shifts caused by  $H'_{A-A}$  may be neglected in some situations depending on the specific model of the bath, the size of the trap, and the number of atoms in the system (for details see [22–24]). We shall omit them in the following, and come back to the discussion of their role in Section VII. We shall therefore postulate a QME restricting our attention to the Liouvillian  $\mathcal{L}$  that describes the cooling process,

$$\mathcal{L} = \sum_{\alpha \neq 0}^{\infty} \mathcal{L}_{\alpha}, \quad (14)$$

where

$$\begin{aligned} \mathcal{L}_{\alpha} \rho_A = & \sum_{\vec{n}, \vec{n}', \vec{m}, \vec{m}'} \Gamma_{\vec{n}, \vec{n}'}^{\vec{m}, \vec{m}'} (2a_{\vec{m}}^{\dagger} a_{\vec{m}'} \rho_A a_{\vec{n}}^{\dagger} a_{\vec{n}'} \\ & - a_{\vec{n}}^{\dagger} a_{\vec{n}'} a_{\vec{m}}^{\dagger} a_{\vec{m}'} \rho_A - \rho_A a_{\vec{n}}^{\dagger} a_{\vec{n}'} a_{\vec{m}}^{\dagger} a_{\vec{m}'}). \end{aligned} \quad (15)$$

The sum in this expression is extended to  $\vec{n}, \vec{n}', \vec{m}, \vec{m}'$  fulfilling

$$\sum_{s=x, y, \dots} (n_s - n'_s) = \alpha, \quad \sum_{s=x, y, \dots} (m_s - m'_s) = -\alpha. \quad (16)$$

Liouvillian (15) accounts for transitions of particles from one level of the harmonic oscillator to another, experiencing a change in the energy of  $\alpha \hbar \omega$ , and a corresponding absorption or emission of a bath quantum. Thus, the term with  $\alpha = 0$  that conserves the energy does not enter (14) since we have excluded the bath quanta with zero energy from the interaction (see Sec. II). The terms with  $\alpha > 0$  ( $\alpha < 0$ ), on the other hand, describe processes increasing (decreasing) the energy. These transitions are characterized by

$$\begin{aligned} \Gamma_{\vec{n}, \vec{n}'}^{\vec{m}, \vec{m}'} = & \frac{\pi}{\hbar} \int d\vec{k} \gamma_{\vec{n}, \vec{n}'}(\vec{k}) \gamma_{\vec{m}, \vec{m}'}^*(\vec{k}) \\ & \times [n(\vec{k}) + 1] \delta[\epsilon(\vec{k}) - \hbar \omega \alpha], \end{aligned} \quad (17)$$

for  $\alpha$  positive, and by

$$\begin{aligned} \Gamma_{\vec{n}, \vec{n}'}^{\vec{m}, \vec{m}'} = & \frac{\pi}{\hbar} \int d\vec{k} \gamma_{\vec{n}, \vec{n}'}(\vec{k}) \gamma_{\vec{m}, \vec{m}'}^*(\vec{k}) \\ & \times n(\vec{k}) \delta[\epsilon(\vec{k}) - \hbar \omega |\alpha|], \end{aligned} \quad (18)$$

for  $\alpha$  negative.

We stress here the fact that for any kind of interactions between the atoms and the bath, the corresponding Liouvillian has the same form as in (14) and (15), provided in each interaction act one atom is annihilated and another created. This is the reason why our results of the following sections can be extended to other kind of interactions. Note, however, that in such cases the coefficients (17) and (18) may have a much more complicated form (see, for example, Ref. [24]).

#### IV. LAMB-DICKE EXPANSION IN 1D

In this Section we perform the Lamb-Dicke (LD) expansion of the master equation (14). From now on we shall concentrate on the one dimensional case and skip the vector notation.

The LD expansion is valid in the situation when the bath quanta relevant for the cooling process have momenta  $\vec{k}$  much smaller than the inverse of the size of

the trap,  $a$ . Their corresponding wave functions  $[\exp(\pm i k x)]$  vary slowly on a scale of  $a$ , and can be then expanded in Taylor series around  $x \simeq 0$ . Since, according to Eqs. (17) and (18) the relevant bath quanta have energies  $\epsilon(k) = \hbar \omega \alpha$ , their corresponding momenta may be determined from the dispersion relation. For example, for the case of massive free particles characterized by the dispersion relation (3), the validity of LD at relatively low temperatures requires that

$$\left( \frac{2M_B \omega |\alpha|}{\hbar} \right)^{1/2} \left( \frac{\hbar}{2M_A \omega} \right)^{1/2} = \left( \frac{M_B |\alpha|}{M_A} \right)^{1/2} < 1, \quad (19)$$

i.e. the effective mass of the bath particles must be much smaller than that of the system atoms [40]. It is easy to find analogous conditions corresponding to other forms of the dispersion relation, including the case of massless bath quanta. In case of the laser cooling (B1) at low temperatures the condition is simply that  $ka = 2\pi a/\lambda < 1$ , where  $k$  ( $\lambda$ ) is the laser photon momentum (wavelength).

In the case of sympathetic cooling (B2) the condition is  $\Delta ka < 1$ , where  $\Delta k$  is the typical momentum transfer in a collision act. In such collision the kinetic energy of the incoming bath atom is of the order of  $1/\beta$ , and its corresponding momentum of the order of  $2\pi/\lambda_B$ , where  $\lambda_B$  denotes the thermal de Broglie wavelength. If the bath was cool,  $\beta \hbar \omega \gg 1$ , the momentum transfer would typically be equal to the final momentum of the bath atom. The validity of LD expansion would then require that the same condition as (19) is fulfilled, with  $M_B$  denoting the real mass of the bath atoms, and that  $2\pi a/\lambda_B < (M_B/M_A)^{1/2} < 1$ .

In the LD regime we can expand the rates (17), (18). Denoting by

$$k_{\alpha} = \left( \frac{2M_B \omega |\alpha|}{\hbar} \right)^{1/2}, \quad (20)$$

$$\eta_{\alpha} = k_{\alpha} a \equiv \sqrt{\alpha} \eta, \quad (21)$$

we obtain for  $n, n', m, m'$  fulfilling Eq. (16)

$$\begin{aligned} \Gamma_{n, n'}^{m, m'} = & \frac{2\pi}{\hbar} \gamma_{n, n'}(k_{\alpha}) \gamma_{m, m'}^*(k_{\alpha}) \\ & \times [n(k_{\alpha}) + (1 + \text{sign}(\alpha))/2] \frac{M_B}{\hbar^2 k_{\alpha}}, \end{aligned} \quad (22)$$

and

$$\begin{aligned} \gamma_{n, n'}(k_{\alpha}) = & \frac{\kappa}{2\pi} \left[ \delta_{n, n'} - i\eta_{\alpha} (\sqrt{n+1} \delta_{n, n'-1} + \sqrt{n} \delta_{n, n'+1}) \right. \\ & - \frac{\eta_{\alpha}^2}{2} (\sqrt{(n+2)(n+1)} \delta_{n, n'-2} + (2n+1) \delta_{n, n'} \\ & \left. + \sqrt{n(n-1)} \delta_{n, n'+2}) + \dots \right] \end{aligned} \quad (23)$$

The master equation can be now rewritten using the above expressions in the interaction picture with respect

to  $H_A$ , and upon neglect of  $H'_{A-A}$ . It takes then the following form

$$\dot{\rho} = \left[ \mathcal{L}^{(0)} + \mathcal{L}_1^{(1)} + \mathcal{L}_2^{(1)} + O(\propto \eta^6) + \dots \right] \rho. \quad (24)$$

The “zeroth” order term is actually of the order of  $\eta^2$  and has the form

$$\begin{aligned} \mathcal{L}^{(0)} \rho = & \Gamma_{\downarrow} [2A\rho A^{\dagger} - A^{\dagger}A\rho - \rho A^{\dagger}A] \\ & + \Gamma_{\uparrow} [2A^{\dagger}\rho A - AA^{\dagger}\rho - \rho AA^{\dagger}]; \end{aligned} \quad (25)$$

where

$$\Gamma_{\downarrow} = N \frac{\kappa^2}{(2\pi)^2} \frac{2\pi}{\hbar} \eta^2 [n(k_1) + 1] \left( \frac{M_B}{\hbar^2 k_1} \right), \quad (26a)$$

$$\Gamma_{\uparrow} = N \frac{\kappa^2}{(2\pi)^2} \frac{2\pi}{\hbar} \eta^2 [n(k_1)] \left( \frac{M_B}{\hbar^2 k_1} \right), \quad (26b)$$

whereas

$$A = \frac{1}{\sqrt{N}} \sum_{n=0}^{\infty} \sqrt{n+1} a_n^{\dagger} a_{n+1}, \quad (27a)$$

$$A^{\dagger} = \frac{1}{\sqrt{N}} \sum_{n=0}^{\infty} \sqrt{n+1} a_{n+1}^{\dagger} a_n. \quad (27b)$$

Note that quite generally: a) both cooling rates  $\Gamma_{\downarrow}, \Gamma_{\uparrow}$  are collective (i.e. proportional to  $N$ ); b) their ratio is

$$\frac{\Gamma_{\uparrow}}{\Gamma_{\downarrow}} = \frac{n(k_1)}{n(k_1) + 1} = z e^{-\beta \hbar \omega}. \quad (28)$$

Similarly, the higher order terms (of order  $\propto \eta^4$ ) are

$$\begin{aligned} \mathcal{L}_1^{(1)} \rho = & -\Gamma_{\downarrow} \eta^2 [2(A\rho C^{\dagger} + C\rho A^{\dagger}) \\ & - (C^{\dagger}A\rho + A^{\dagger}C\rho) - (\rho C^{\dagger}A + \rho A^{\dagger}C)] \\ & -\Gamma_{\uparrow} \eta^2 [2(A^{\dagger}\rho C + C^{\dagger}\rho A) \\ & - (CA^{\dagger}\rho + AC^{\dagger}\rho) - (\rho CA^{\dagger} + \rho AC^{\dagger})], \end{aligned} \quad (29)$$

with

$$C = \frac{1}{2\sqrt{N}} \sum_{n=0}^{\infty} (n+1)^{3/2} a_n^{\dagger} a_{n+1}, \quad (30a)$$

$$C^{\dagger} = \frac{1}{2\sqrt{N}} \sum_{n=0}^{\infty} (n+1)^{3/2} a_{n+1}^{\dagger} a_n, \quad (30b)$$

and

$$\begin{aligned} \mathcal{L}_2^{(1)} \rho = & \Gamma_{\downarrow}^{(1)} [2B\rho B^{\dagger} - B^{\dagger}B\rho - \rho B^{\dagger}B] \\ & + \Gamma_{\uparrow}^{(1)} [2B^{\dagger}\rho B - BB^{\dagger}\rho - \rho BB^{\dagger}]; \end{aligned} \quad (31)$$

where

$$\Gamma_{\downarrow}^{(1)} = N \frac{\kappa^2}{(2\pi)^2} \frac{2\pi}{\hbar} \frac{\eta_2^4}{4} [n(k_2) + 1] \left( \frac{M_B}{\hbar^2 k_2} \right), \quad (32a)$$

$$\Gamma_{\uparrow}^{(1)} = N \frac{\kappa^2}{(2\pi)^2} \frac{2\pi}{\hbar} \frac{\eta_2^4}{4} [n(k_2)] \left( \frac{M_B}{\hbar^2 k_2} \right), \quad (32b)$$

whereas

$$B = \frac{1}{\sqrt{N}} \sum_{n=0}^{\infty} \sqrt{(n+1)(n+2)} a_n^{\dagger} a_{n+2}, \quad (33a)$$

$$B^{\dagger} = \frac{1}{\sqrt{N}} \sum_{n=0}^{\infty} \sqrt{(n+1)(n+2)} a_{n+2}^{\dagger} a_n. \quad (33b)$$

Note that similarly as in Eq. (28) the rates fulfill

$$\frac{\Gamma_{\uparrow}^{(1)}}{\Gamma_{\downarrow}^{(1)}} = \frac{n(k_2)}{n(k_2) + 1} = z e^{-2\beta \hbar \omega}. \quad (34)$$

Finally, Eq. (24) contains terms of higher orders  $\propto \eta^6, \eta^8$ , etc.

## V. ACCIDENTAL DEGENERACY AND THE BREAKDOWN OF ERGODICITY

In this Section we discuss the dynamics governed by the lowest order term in the Lamb-Dicke expansion, i.e. by the equation

$$\dot{\rho} = \mathcal{L}^{(0)} \rho. \quad (35)$$

First we observe that

$$[A, A^{\dagger}] = 1, \quad (36)$$

i.e. the operators  $A$ , and  $A^{\dagger}$  represent an abstract harmonic oscillator Weyl–Heisenberg algebra, whereas the Liouville-von Neuman superoperator (25) describes *interaction of that harmonic oscillator with an effective thermal bath* (see, for instance [21]). The inverse temperature of the bath is given by

$$\hbar \omega \beta_e = -\log \left( \frac{\Gamma_{\uparrow}}{\Gamma_{\downarrow}} \right) = \hbar \omega \beta - \beta \mu. \quad (37)$$

Note that the effective temperature is never greater than the temperature of the bath,  $\beta_e \geq \beta$ , since  $\mu \leq 0$ . Alternatively, one may view the above equation, as if the effective temperature of the system was constant, but the frequency would change  $\hbar \omega_e = \hbar \omega - \mu$ . This effect is a result of our definition of the system–bath interactions. Those interactions consist of absorption or emission of the bath quanta, and thus do not conserve the number of the bath particles. The Boltzmann exponent (37) must account for energy gain or loss due to bath particles creation/annihilation. The remaining question is how the abstract operator algebra is represented in the Fock-Hilbert space of our multiparticle system. To answer this question we first introduce the operator

$$D = B - A^2/\sqrt{N}, \quad (38)$$

which commutes with  $A, A^{\dagger}, B$  and  $B^{\dagger}$ . We then observe that (see appendix A):

- For each value of  $l = 0$ , or  $l = 2, 3, \dots$  there exist  $n_N(l)$ , so called, *vacuum* states  $|0_{lsv}\rangle$  that are annihilated by the “jump” operator  $A = \sum_{n=0}^{\infty} \sqrt{n+1} g_n^\dagger g_{n+1}$ ,

$$A|0_{lsv}\rangle = 0, \quad (39)$$

where the index  $l$  indicates the *bare energy* of the corresponding states (in units of  $\hbar\omega$ ),

$$\sum_{n=0}^{\infty} n a_n^\dagger a_n |0_{l,s}\rangle = l |0_{l,s}\rangle, \quad (40)$$

The state corresponding to  $l = 0$  contains all  $N$  atoms in the ground state. The states with higher energy are constructed as linear combinations of degenerated Fock states. There is only one state of  $l = 1$  ( $N - 1$  atoms in the ground state, and one atom in the first excited state), which is not annihilated by  $A$ ; that is why there is no vacuum state with  $l = 1$ . The index  $s$  measures the number of excitations of  $D^\dagger$  in the state  $|0_{lsv}\rangle \propto (D^\dagger)^s |0_{l-2s0v}\rangle$ , and runs from 0 to  $E(l/2)$ , i.e. integer part of  $l/2$ . Each of the states  $|0_{lsv}\rangle$  is an eigenstate of  $D^\dagger D$  with an eigenvalue  $(4ls - 4s^2 - 2s + 2Ns)/N$ . The index  $v$  enumerates finally the states of energy  $l - 2s$  annihilated by  $D$ . Denoting by  $m_N(l)$  the number of states of energy  $l$  annihilated by  $D$ , i.e. the states

$$D|0_{l0v}\rangle = 0, \quad (41)$$

we obtain

$$n_N(l) = \sum_{s=0}^{E(l/2)} m_N(l - 2s). \quad (42)$$

The construction of the vacuum states is described in the Appendix A. Some other examples of the vacua are constructed in Appendix B. Each of the vacuum states is a linear combination of the *accidentally degenerated* energy eigenstates. The number of accidentally degenerated states of the energy  $l$  in the  $N$  atom system,  $p_N(l)$ , is given by a solution of the partition problem of the number theory [41] and is extravagantly large (c.f.  $p_N(l) \simeq O(\exp(\pi\sqrt{2l/3}))$  for  $l \leq N$ ). The number of the vacua is given by  $n_N(l) = p_N(l) - p_N(l - 1)$ . The very existence of these multiple vacuum states is thus a direct consequence and, at the same time, a signature of the *accidental degeneracy* [42].

- The vacuum states are orthonormal,  $\langle 0_{lsv} | 0_{l's'v'} \rangle = \delta_{ll'} \delta_{ss'} \delta_{vv'}$ .
- The Fock-Hilbert space of the system splits into an infinite number of Fock subspaces corresponding to each of the vacuum states. The Fock states in the  $(l, s, v)$ -th subspace are constructed as

$$|k_{lsv}\rangle = \frac{(A^\dagger)^k}{\sqrt{k!}} |0_{lsv}\rangle, \quad (43)$$

with  $k = 0, 1, \dots$ . They are also mutually orthonormal, and are also eigenstates of the energy operator with the corresponding eigenvalue  $(l + k)$ . They are also highly degenerated (for  $k + l = k' + l'$ ). In the following we shall use the notation  $w = (l, s, v)$ .

The dynamics exhibits in the Lamb-Dicke limit multiple timescales. On the fastest time scale of the order of  $\eta^{-2}$  it is *nonergodic*, i.e. it does not mix the different  $w$ -subspaces. After a short time of the order of the inverse of  $\Gamma_\downarrow$ ,  $\Gamma_\uparrow$  all coherences between the  $|k_w\rangle$  and  $|k'_{w'}\rangle$  for  $k \neq k'$  vanish. Within each  $w$ -subspace the system approaches the “thermal” equilibrium characterized by the density matrix diagonal in  $k$ , with zero off-diagonal elements, and the inverse temperature  $\beta_e$ . The dynamics, however, *cannot be reduced to a Poisson jump process*, i.e. a sequence of random jumps between the various  $|k_w\rangle$  states with the transition probabilities governed by the detailed balance conditions characteristic for the thermal equilibrium. The reason is that coherences corresponding to  $w \neq w'$ , but  $k = k'$  do not vanish.

The quantum mechanical density matrix in this (formally stationary) limit becomes a sum of diagonal *canonical ensembles* in each of the subspaces, accompanied by a sum of non-diagonal terms connecting different  $w$  and  $w'$  for the same  $k$ 's,

$$\rho = [1 - \exp(-\beta_e \hbar\omega)] \sum_w \sum_k n_w |k_w\rangle \langle k_w| e^{-\beta_e \hbar\omega k} + [1 - \exp(-\beta_e \hbar\omega)] \sum_{w \neq w'} \sum_k r_{ww'} |k_w\rangle \langle k_{w'}| e^{-\beta_e \hbar\omega k}. \quad (44)$$

where the coefficients describe the populations of the corresponding subspaces, and are defined as

$$n_w = \text{Tr}(P_w \rho(0) P_w), \quad (45)$$

and the cumulative coherences,

$$r_{ww'} = \sum_k \langle k_w | \rho(0) | k_{w'} \rangle. \quad (46)$$

Evidently,  $\rho$  exhibits nonergodic effects and depends explicitly on the initial density operator. In the above expression  $P_w = \sum_k |k_w\rangle \langle k_w|$  denotes a projection operator onto the  $w$ -th subspace. Note that the definition (45) implies that  $\sum_w n_w = 1$ .

We stress that in the Fock basis spanned by the states  $|k_w\rangle$  the matrix  $\rho$  is, in principle, not diagonal; moreover, in general, depending on the initial condition, it does contain coherences when represented in the Fock-Hilbert space corresponding to noninteracting atoms. That is the reason why the master equation in the latter basis cannot be reduced to the diagonal form in the Lamb-Dicke limit. That is why in order to arrive at such reduction additional assumptions have to be evoked that lift up the



accidental degeneracy, as anharmonicity of energy levels caused by anharmonicity of the trap potential or interatomic interactions.

## VI. RESTORATION OF ERGODICITY

From the previous Section it is clear that the breakdown of ergodicity has only an approximate character since it is related to the lowest order dynamics in the LD expansion. It is natural to expect that Eq. (44) describes only a quasi-stationary solution which is indeed reached on a time scale  $1/\Gamma_\uparrow, 1/\Gamma_\downarrow \simeq O(\propto 1/\eta^2)$ , but undergoes further slow evolution on a time scale  $1/\Gamma_\uparrow^{(1)}, 1/\Gamma_\downarrow^{(1)} \simeq O(\propto 1/\eta^4)$ . On this slower time scale the ergodicity should be (at least partially) restored, and the transitions between the different  $w$ -th subspaces should become possible. As we shall see below, that is indeed the case.

To this aim we consider the higher order corrections to the master equation (24) and treat them perturbatively within the standard adiabatic elimination method [43]. We introduce the projection operator

$$\mathcal{P}\rho(t) = \sum_w n_w(t) \sum_k |k_w\rangle\langle k_w| e^{-\beta_e \hbar \omega k} (1 - e^{-\beta_e \hbar \omega}) + \sum_{w \neq w'} r_{ww'}(t) \sum_k |k_w\rangle\langle k_{w'}| e^{-\beta_e \hbar \omega k} (1 - e^{-\beta_e \hbar \omega}), \quad (47)$$

where the populations of the corresponding subspaces

$$n_w(t) = \text{Tr}(P_w \rho(t) P_w), \quad (48)$$

and the cumulative coherences

$$r_{ww'}(t) = \sum_k \langle k_w | \rho(t) | k_{w'} \rangle, \quad (49)$$

become now slowly varying functions of time.

Introducing the complementary projector  $\mathcal{Q} = 1 - \mathcal{P}$  obtain

$$\dot{\mathcal{P}}\rho = \mathcal{P}(\mathcal{L}_1^{(1)} + \mathcal{L}_2^{(1)})\mathcal{P}\rho + \mathcal{P}(\mathcal{L}_1^{(1)} + \mathcal{L}_2^{(1)})\mathcal{Q}\rho, \quad (50)$$

$$\dot{\mathcal{Q}}\rho = \mathcal{Q}\mathcal{L}^{(0)}\mathcal{Q}\rho + \mathcal{Q}(\mathcal{L}_1^{(1)} + \mathcal{L}_2^{(1)})\mathcal{P}\rho + \dots \quad (51)$$

In the latter Eq. (51) we have already employed the fact that  $\Gamma^{(1)}/\Gamma \simeq O(\propto \eta^2)$ , and neglected the higher order terms in  $\eta^2$ . Moreover, adiabatic elimination of  $\mathcal{Q}\rho$  from Eq. (51) introduces corrections of the order  $\propto \eta^6$  to Eq. (50) for  $\mathcal{P}\rho$ . Thus it may also be neglected in comparison to the leading term on the RHS of Eq. (50).

We obtain thus a relatively simple master equation

$$\dot{\mathcal{P}}\rho = \mathcal{P}(\mathcal{L}_1^{(1)} + \mathcal{L}_2^{(1)})\mathcal{P}\rho \quad (52)$$

From this master equation, after elementary algebra we obtain a set of closed rate equations for the populations  $n_w$  of the  $w$ -th subspaces, and the coherences  $r_{ww'}$ . These equations can be enormously simplified using the properties of the operators  $A$ ,  $B$ ,  $C$ , and their hermitian conjugates that are discussed in Appendix A. Amazingly, it is only the term  $\mathcal{L}_2^{(1)}$  which contributes in this order of the LD expansion; moreover, the equations for populations and coherences decouple (see Appendix C for details),

$$\begin{aligned} \dot{n}_w = & 2\Gamma_\downarrow^{(1)}(1 - e^{-\beta_e \hbar \omega}) \sum_k \left( \sum_{k', w'} |\langle k_w | B | k_{w'}' \rangle|^2 e^{-\beta_e \hbar \omega k'} n_{w'} - \langle k_w | B^\dagger B | k_w \rangle e^{-\beta_e \hbar \omega k} n_w \right) \\ & + 2\Gamma_\uparrow^{(1)}(1 - e^{-\beta_e \hbar \omega}) \sum_k \left( \sum_{k', w'} |\langle k_w | B^\dagger | k_{w'}' \rangle|^2 e^{-\beta_e \hbar \omega k'} n_{w'} - \langle k_w | B B^\dagger | k_w \rangle e^{-\beta_e \hbar \omega k} n_w \right), \end{aligned} \quad (53)$$

$$\begin{aligned} \dot{r}_{ww'} = & 2\Gamma_\downarrow^{(1)}(1 - e^{-\beta_e \hbar \omega}) \sum_k \left( \sum_{k', w_1, w_2} \langle k_w | B | k_{w_1}' \rangle \langle k_{w_2}' | B^\dagger | k_{w'} \rangle e^{-\beta_e \hbar \omega k'} r_{w_1 w_2} \right. \\ & \left. - \frac{1}{2} \sum_{w_1} [\langle k_w | B^\dagger B | k_{w_1} \rangle r_{w_1 w'} + \langle k_{w_1} | B^\dagger B | k_{w'} \rangle r_{w w_1}] e^{-\beta_e \hbar \omega k} \right) \\ & + 2\Gamma_\uparrow^{(1)}(1 - e^{-\beta_e \hbar \omega}) \sum_k \left( \sum_{k', w_1, w_2} \langle k_w | B^\dagger | k_{w_1}' \rangle \langle k_{w_2}' | B | k_{w'} \rangle e^{-\beta_e \hbar \omega k'} r_{w_1 w_2} \right. \\ & \left. - \frac{1}{2} \sum_{w_1} [\langle k_w | B B^\dagger | k_{w_1} \rangle r_{w_1 w'} + \langle k_{w_1} | B B^\dagger | k_{w'} \rangle r_{w w_1}] e^{-\beta_e \hbar \omega k} \right), \end{aligned} \quad (54)$$

The above equations are further reduced inserting the unity between  $B$  and  $B^\dagger$ , and using the fact that  $A$ , and  $A^\dagger$  by definition do not couple the different  $w$ -subspaces, whereas  $B$  ( $B^\dagger$ ) has the only relevant matrix elements between the different  $lsv$ -subspaces for the  $(l \pm 2, s \pm 1, v)$ -th and  $lsv$ -th subspace, for  $l = 2, 3, \dots$  ( $l = 0, 2, 3, \dots$ ),  $s = 0, \dots, E(l/2)$ , and  $k = k' = 0, 1, \dots$  (see Appendix C).

From the above considerations we obtain the final form of the equations

$$\dot{n}_w = 2\Gamma_\downarrow^{(1)} [f_{w+2}^2 n_{w+2} - f_w^2 n_w] + 2\Gamma_\uparrow^{(1)} [f_w^2 n_{w-2} - f_{w+2}^2 n_w]. \quad (55)$$

$$\dot{r}_{ww'} = 2\Gamma_\downarrow^{(1)} \left[ f_{w+2} f_{w'+2} r_{w+2w'+2} - \frac{1}{2} (f_w^2 + f_{w'}^2) r_{ww'} \right] + 2\Gamma_\uparrow^{(1)} \left[ f_w f_{w'} r_{w-2w'-2} - \frac{1}{2} (f_{w+2}^2 + f_{w'+2}^2) r_{ww'} \right], \quad (56)$$

where we have denoted  $w = (lsv)$ ,  $w \pm 2 = (l \pm 2, s \pm 1, v)$ , with  $f_w = \langle 0_{w-2} | B | 0_w \rangle$ . Note that  $f_w$  can be assumed to be real and positive without loss of generality. As we see, both the populations  $n_w$ , and the coherences  $r_{ww'}$  fulfill a closed set of *rate equations*. The explicit expressions for the matrix elements involved in the above formulae are derived in Appendix C.

The above equations provide the basic result of this paper. It shows that due to the presence of accidental degeneracy in the LDL the dynamics occurs essentially on several time scales. On the fastest time scale (governed by  $\mathcal{L}^{(0)}$ ) the dynamics is nonergodic and consist in approach toward the canonical equilibrium states in each of the  $l$ -subspaces, accompanied by creation of quasi-equilibrium coherences between the states corresponding to the same  $k$ 's, but different  $w$  and  $w'$ . On this scale the populations of each of the  $w$ -subspace, as well as the cumulative coherences  $r_{ww'}$  may be regarded as constant, and therefore the values of these coherences, as well as the populations in each of the subspaces depend on the initial conditions. In the higher order of expansion (on the time scale  $1/\eta^2$  times longer), the mixing between different  $w$ -subspaces becomes possible. This mixing leads to a partial restoration of ergodicity. In the example considered here this restoration is not full, however, because as easily seen from Eq. (55) the  $w$ -subspaces with different  $v$  still do not mix. The reader can easily check that the further mixing of the odd and even subspaces does take place in the next order of the Lamb-Dicke expansion (for instance due to term containing bi-products of the operators  $C$ , and  $C^\dagger$ ).

The stationary state that is reached on the slower time scale is easy to find since Eqs. (55) fulfill the detailed balance conditions, whereas the cumulative coherences are damped to zero, as demonstrated in Appendix D. We obtain that

$$n_{l+2,s+1,v} = z e^{-2\beta\hbar\omega} n_{lsv}, \quad (57)$$

so that

$$n_{2l+m,l,v} = e^{-2\beta'_e \hbar\omega l} n_{m0v}, \quad (58)$$

with

$$\beta'_e = \beta - \beta\mu/2\hbar\omega. \quad (59)$$

The ratio of  $n_{m0v}$ , and  $n_{m'0v'}$  remain undetermined in this order. Note that the reason why  $\beta'_e \neq \beta_e$  is that both temperatures correspond to the processes that involve single bath quantum absorption or emission, but different energy changes (by  $\hbar\omega$ , or  $2\hbar\omega$ , respectively). Indeed, it is elementary to check that the stationary diagonal matrix elements of the density matrix are proportional to the corresponding Boltzmann factors,

$$\langle k_{2l+m,l,v} | \rho | k_{2l+m,l,v} \rangle \propto e^{-\beta_e \hbar\omega k - 2\beta'_e \hbar\omega l} n_{m0v} = \langle k_{2l+m,l,v} | e^{-\beta'_e \hbar\omega \hat{E} - m + \beta\mu A^\dagger A/2} n_{m0v} | k_{2l+m,l,v} \rangle. \quad (60)$$

Finally, it is easy to check by substitution in the Liouillian (14) that for  $\mu = 0$  the steady state to all orders in the LD expansion is precisely  $\rho \propto e^{-\beta H_A}$ , which is diagonal in the original basis. Obviously, the steady state solutions obtained in the first, and the second order of our expansion are compatible with such a steady state.

## VII. CONCLUSIONS

In a series of papers [22–24,27] we have studied in detail the quantum dynamics of bosonic and fermionic gases of cold atoms in traps in the absence of accidental degeneracy. We studied various cooling mechanism, and various limiting cases. In this paper we have presented the solution of the corresponding problem accounting for accidental degeneracy effects. We have studied interactions of a gas of trapped atoms with a heat bath in the Lamb-Dicke limit using the master equation approach. We have demonstrated that the system approaches an equilibrium on two (or more) distinguished time scales, and that the dynamics has the corresponding number of stages. At each stage a *quasi-equilibrium* state within appropriately determined subspaces of the Hilbert space is reached. This quasi-equilibrium corresponds to a canonical ensemble restricted to the appropriate subspace, and characterized by an effective temperature determined by the temperature and the chemical potential of the heat bath. In the next stage thermalization between the groups of subspaces occurs leading to another quasi-equilibrium in the larger subspaces, and so on.

We would like to stress once more that the problem considered in this paper is quite general. Atomic traps, although frequently anisotropic (see for example Ref. [3]), can be designed to be harmonic with a very good accuracy. A cooled atomic sample in such a harmonic microtrap will necessarily exhibit the effects of accidental degeneracy *regardless of the method used for its cooling!*

One may question the generality of our results, since we have used the Lamb-Dicke expansion, and at the same time neglected in this paper atom-atom collisions, as well as atom-atom interactions mediated by the coupling with the bath. Such processes (described by the Hamiltonian  $H'_{A-A}$ , see Section III) lead evidently to shifts of the atomic energy levels, and will, in principle, lift up the accidental degeneracies. As we argued in Refs. [22–24], as long as the number of atoms in the microtrap is not too large, those shifts remain small and can be treated perturbatively. The system will then still exhibit the effects of accidental quasi-degeneracy. We stress that the theory developed in this article is valid for arbitrary numbers of atoms, and in particular it is for two atoms. Using far-off-resonance dipole traps [44], or loading atoms to a single minimum of a dark optical lattice (see Ref. [6](b)) it should be accessible experimentally to confine several atoms in the trap of the size  $a \simeq 0.1 - 0.05 \mu\text{m}$ . That implies validity of the LD expansion for the laser colling case (see [22]). Similarly, one can use a cooled atomic gas close to, or below the condensation point as a bath in the symphatetic cooling case. In the conditions of the experiments of Refs. [3] and [5] that implies de Broglie wavelength of the order of  $\mu\text{m}$ , and thus validates the LD expansion. Using Bogoliubov-Hartree theory it is possible to estimate perturbatively that the energy level splittings in a "band" of the quasi-degenerated states due to atom-atom collisions will be in such a case of the order of  $N(a_{sc}/a)/\sqrt{N_D}$ , where  $a_{sc}$  is the scattering length of the system atoms, and  $N_D$  is the number of levels in the band. Note that  $N_D$  increases dramatically for higher excited levels. We see with  $a_{sc} = 5 \text{ nm}$ , our theory should work for  $N$  up to  $\simeq 20$  even in the worst case when  $N_D = 2$ . Note that the cooling of 20 atoms to the ground state of a harmonic trap might be a very interesting task for the rapidly-developing research field of quantum informacion processing. Additionally, we want to recall at this point that as pointed above, the external modification of the  $s$ -wave scattering length via Feshbach resonances has been demonstrated, been experimentally feasible the achievement of a quasi-ideal gas.

The main physical results of the paper are thus the following. We have been able to treat analytically the quantum dynamics of an ideal gas of  $N$  atom in the LD limit. We have shown that the dynamics naturally splits into two parts: a fast part, during which coherences between the degenerated states are preserved, and a slower part, during which thermal equilibrium is achieved. Even though, the ideal case considered is not realistic (at least without external modification of the scattering length), we think i) that it provides a lot of insight into more realistic situations; ii) it is, to our knowledge, one of the extremely rare examples of soluble quantum dynamical problems in the area of statistical physics. The method that we developed, and results can be carried over to more realistic situations concerning cooling of small atomic samples ( $\simeq 20$  atoms) in microtraps. Such situations are not far from the reach of present exper-

iments. The calculations for such a case should follow exactly the lines described in this paper, with the only difference that the parts of the Liouville equations describing the atom-atom interactions that lift up the exact degeneracies should be included into the corrections to the  $\mathcal{L}^{(0)}$ . In another words, they should be treated just like the corrections to the lowest order term in the LD expansion have been treated in this paper. It is obvious, that as long as the splittings of the quasi-degenerated levels will remain small relative to  $\hbar\omega$ , such realistic system will exhibit basic effects presented in this paper, i.e. step-wise dynamics on the two time scales.

The quantum dynamics of samples of cold atoms exhibits, in our opinion, an enormous reachness of interesting physical and mathematical phenomena, such as multistable, exotic stationary states, multistage dynamics etc. The present paper is another example of this reachness. Further studies are, however, required to get more understanding of this new physics, including for instance developement of other statistical physics tools [28](c), such as diffusion equations, hydrodynamic limits etc.

After this work was finished we have learned from T. Fischer, K. Vogel and W. Schleich that similar algebra to the one used by us appears in the problem of the cooling of a sample of bosons with a simple particle reservoir [45]. We thank Yvan Castin, Jean Dalibard, Ralph Dum, T. Fischer, K. Vogel, and P. Zoller for enlighting discussions. We acknowledge the support of the Deutsche Forschungsgemeinschaft (SFB 407), ESF PESC Proposal BEC2000+, and TMR ERBXTCT96-0002.

## APPENDIX A: THE STRUCTURE OF THE FOCK-HILBERT SPACE

The matrix elements of the operators  $B$ , and  $C$  can be calculated using elegant algebraic methods. To this aim we first observe that the operators in question fulfill the commutation relations

$$[A, B] = 0, \quad (\text{A1a})$$

$$[A, C] = B/(2\sqrt{N}), \quad (\text{A1b})$$

$$[A, B^\dagger] = 2A^\dagger/\sqrt{N}, \quad (\text{A1c})$$

$$[A, C^\dagger] = \hat{E}/N + 1/2, \quad (\text{A1d})$$

$$[B, B^\dagger] = 4\hat{E}/N + 2, \quad (\text{A1e})$$

$$[B, \hat{E}] = 2B, \quad (\text{A1f})$$

$$[C, \hat{E}] = C, \quad (\text{A1g})$$

$$[A, \hat{E}] = A, \quad (\text{A1h})$$

with  $\hat{E} = \sum_{n=0}^{\infty} n a_n^\dagger a_n$  denoting the normalized energy operator.

It proves to be very useful to introduce the operator

$$D = B - A^2/\sqrt{N}. \quad (\text{A2})$$

This operator fulfills

$$[D, A] = 0, \quad (\text{A3a})$$

$$[D, A^\dagger] = 0, \quad (\text{A3b})$$

$$[D, D^\dagger] = 4(\hat{E} - A^\dagger A)/N + 2(1 - 1/N), \quad (\text{A3c})$$

Since the operators  $A^\dagger A$ , and  $D^\dagger D$  commute, it is useful to characterize the multiple vacua in terms of the eigenvalues of these two hermitian operators.

Let  $|0_{lv}\rangle$  denote the states that fulfill

$$A|0_{lv}\rangle = 0, \quad (\text{A4a})$$

$$D|0_{lv}\rangle = 0. \quad (\text{A4b})$$

There are  $m_N(l)$  such states, and the index  $v$  enumerates them. Note that the states

$$|0_{lsv}\rangle = (D^\dagger)^s |0_{l-2s,0,v}\rangle / \|(D^\dagger)^s |0_{l-2s,0,v}\rangle\|, \quad (\text{A5})$$

have energy  $l$ , are annihilated by  $A$ , and are eigenstates of  $D^\dagger D$  with the eigenvalue

$$\sum_{s'=0}^{s-1} [4(l - 2s + 2s')/N + 2(1 - 1/N)]. \quad (\text{A6})$$

In the subsequent energy sectors we have thus the vacua:  $|0_{001}\rangle$ ,  $|0_{211}\rangle$ ,  $|0_{301}\rangle$ ,  $|0_{421}\rangle$ ,  $|0_{401}\rangle$ ,  $|0_{511}\rangle$ ,  $|0_{501}\rangle$ ,  $|0_{631}\rangle$ ,  $|0_{611}\rangle$ ,  $|0_{601}\rangle$ ,  $|0_{602}\rangle$ , etc.

The Fock-Hilbert space is spanned by the vectors

$$|k_{lsv}\rangle = \frac{(A^\dagger)^k}{\sqrt{k!}} |0_{lsv}\rangle. \quad (\text{A7})$$

## APPENDIX B: CONSTRUCTION OF VACUUM STATES

We have seen in Appendix A that the vacuum states can be constructed by applying the operator  $D^\dagger$  consecutively to the states  $|0_{l,0,v}\rangle$ . In this Appendix we present explicit construction of another family of the vacuum states that are annihilated by the operator  $A$ . In fact we consider a more general case with

$$A = \sum_{n=0} A_n a_n^\dagger a_{n+1}. \quad (\text{B1})$$

Such defined operator reduces to the one given by Eq. (27a) if we put  $A_n = \sqrt{n+1}$ . The vacuum states fulfill

$$A|0_l\rangle = 0 \quad (\text{B2})$$

There is one obvious solution of the above equation which describes the global ground state

$$|0_0\rangle = |N, 0, 0, \dots\rangle. \quad (\text{B3})$$

Apart from that, for  $l = 2, 3, \dots$  we define

$$|0_l\rangle = \sum_{m=1}^{l-1} \alpha_m^l a_{l+1-m}^\dagger |N - m, m - 1, 0, \dots\rangle + \alpha_l^l |N - l, l, 0, \dots\rangle. \quad (\text{B4})$$

From the above definition it is clear, that different vacua are orthogonal. Applying  $A$  to the above expression after elementary algebra we derive the recurrence formulas for the coefficients

$$\alpha_m^l = -\frac{A_0}{A_{l-m}} \sqrt{m} \sqrt{N - m} \alpha_{m+1}^l \quad (\text{B5})$$

valid for  $m = 1, l - 2$ , and

$$\alpha_{l-1}^l = -\frac{A_0}{A_1} \frac{\sqrt{l} \sqrt{N - l + 1}}{\sqrt{l - 1}} \alpha_l^l. \quad (\text{B6})$$

From the above expression it is easy to construct explicitly the corresponding vacuum states. The value of  $\alpha_l^l$  can be conveniently chosen for normalisation of the states.

In the case considered in this paper ( $A_n = \sqrt{n+1}$ ) the first few normalized vacuum states are:

$$|0_2\rangle = \frac{1}{\sqrt{N}} (|N - 2, 2, 0, \dots\rangle - \sqrt{N-1} |N - 1, 0, 1, 0, \dots\rangle), \quad (\text{B7})$$

$$|0_3\rangle = \frac{\sqrt{8}}{\sqrt{N^2 + 3N - 2}} (|N - 3, 3, 0, \dots\rangle - \frac{\sqrt{3(N-2)}}{2} |N - 2, 1, 1, 0, \dots\rangle + \frac{\sqrt{(N-1)(N-2)}}{2\sqrt{2}} |N - 1, 0, 0, 1, 0, \dots\rangle) \quad (\text{B8})$$

$$|0_4\rangle = \frac{3}{\sqrt{N^3 - 5N^2 - 3N + 21}} (|N - 4, 4, 0, \dots\rangle - \frac{\sqrt{2(N-3)}}{3} |N - 3, 2, 1, 0, \dots\rangle + \frac{2\sqrt{(N-2)(N-3)}}{3} |N - 2, 1, 0, 1, 0, \dots\rangle - \frac{\sqrt{(N-1)(N-2)(N-3)}}{3} |N - 1, 0, 0, 0, 1, 0, \dots\rangle) \quad (\text{B9})$$

etc.

## APPENDIX C: CALCULATION OF THE MATRIX ELEMENTS

Let us first consider the operator  $B$ , and derive the explicit expressions for the matrix elements

$$f_{lsv} = \langle 0_{l-2s-1v} | B | 0_{lsv} \rangle = \langle 0_{l-2s-1v} | D | 0_{lsv} \rangle \quad (C1)$$

that enter Eq. (55). Note that the coefficients  $f_{lsv}$  are real, since the matrix elements of the operator  $A$  in the non-interacting atom basis are real (see Appendix A). Moreover, without any loss of generality  $f_{lsv}$ 's may be assumed to be non-negative. In the following I will skip the index  $v$  which is not affected by the dynamics.

Since we know that  $B|0_{ls}\rangle \propto |0_{l-2s-1}\rangle$  for  $l \geq 2s$ , we can write

$$B|0_{ls}\rangle = f_{ls}|0_{l-2s-1}\rangle. \quad (C2)$$

Similarly, using the commutation relation (A1c) we can write

$$B^\dagger|0_{l-2s-1v}\rangle = f_{ls}|0_{ls}\rangle + \sqrt{2/N}|2_{l-2,s}\rangle, \quad (C3)$$

or

$$f_{ls}^2 = \langle 0_{l-2,s-1} | BB^\dagger | 0_{l-2,s-1} \rangle - 2/N. \quad (C4)$$

From the above expressions using the commutation relation (A1e) we obtain

$$f_{l+2,+1}^2 = f_{ls}^2 + 4l/N + 2 - 2/N. \quad (C5)$$

The above recurrence can be easily solved yielding

$$f_{ls}^2 = (2 - 2/N)s + 4((l - 2s)s + s(s - 1))N. \quad (C6)$$

since  $f_{l-2s,0} = 0$ .

In general, we may write

$$B|k_{ls}\rangle = f_{ls}|k_{l-2,s-1}\rangle + \sqrt{k(k-1)/N}|(k-2)_{ls}\rangle. \quad (C7)$$

The above formulae provide a very efficient method of calculating all of the matrix elements of the operators  $B$  and  $B^\dagger$ .

It is a little more tedious to derive corresponding formulae for the operator  $C$ . From Eq. (A1a) we obtain

$$AC|0_{ls}\rangle = \frac{1}{2\sqrt{N}}f_{ls}|0_{l-2,s-1}\rangle, \quad (C8)$$

so that

$$C|0_{ls}\rangle = \frac{1}{2\sqrt{N}}f_{ls}|1_{l-2,s-1}\rangle + \sum_{s'}^{E(l-1/2)} w_{ls'}|0_{l-1,s'}\rangle. \quad (C9)$$

The coefficients  $w_{ls'} = \langle 0_{l-1,s-1} | C | 0_{ls} \rangle$  may be also regarded to be real, and can be, for instance, determined directly from the definitions of the vacuum states.

In general, we can write

$$C|k_{ls}\rangle = \frac{\sqrt{k+1}}{2\sqrt{N}}f_{ls}|k+1_{l-2,s-1}\rangle + \sum_{s'}^{E(l-1/2)} w_{ls'}|k_{l-1,s'}\rangle + v_{ls}(k)|k-1_{ls}\rangle, \quad (C10)$$

with

$$v_{ls}(k+1) = \sqrt{\frac{k}{k+1}}v_{ls}(k) + \frac{1}{\sqrt{k+1}}\left(\frac{k+l}{N} + \frac{1}{2}\right), \quad (C11)$$

and  $v_{ls}(0) = 0$ . The above formulae allow for very efficient calculations of the matrix element of the operators  $C$  and  $C^\dagger$ , provided the states  $|0_{m0v}\rangle$  are known.

The expression (C10) implies immediately that  $\mathcal{L}_1^{(1)}$  does not contribute at all to the final equations (54) and (54). Since the matrix  $\rho$  is diagonal in the  $k$  index, whereas the operators  $A$  and  $A^\dagger$  change  $k$  to  $k-1$ , and  $k+1$  respectively, only those parts of the operators  $C$  and  $C^\dagger$  that change  $k \pm 1$  back to  $k$  could contribute. It is evident from Eq. (C10), however, that these parts of  $C$  and  $C^\dagger$  do not change  $lsv$ . Therefore, their contributions to Eqs. (54) and (54) vanish identically, due to the trace-like sums over  $k$  appearing on the right hand side.

Similar considerations show that there is no mixing of the populations and the cumulative coherences in Eqs. (54) and (54). Let us, for example, consider Eq. (54) for the populations  $n_{lsv}$ . As in the previous case, the contributions of the parts of the operators  $B$  and  $B^\dagger$  that do not change  $lsv$  vanish identically, due to the trace-like sums over  $k$  appearing on the right hand side. The parts of  $B$  and  $B^\dagger$  that change  $l$  by  $\mp 2$ , and  $s$  by  $\mp 1$  do contribute, but they can only transform the parts of the density matrix proportional to  $|k_{lsv}\rangle\langle k_{l's'v'}|$  into  $\propto |k_{lsv}\rangle\langle k_{l's'v'}|$ , or  $\propto |k_{l\pm 2,s\pm 1,v}\rangle\langle k_{l'\pm 2,s'\pm 1,v'}|$ , i.e. they can only lead to couplings between the populations  $n_{lsv}$  and  $n_{l\pm 2,s\pm 1,v}$ , or between the cumulative coherences  $r_{lsv,l's'v'}$  and  $r_{l\pm 2,s\pm 1,v,l'\pm 2,s'\pm 1,v'}$ .

## APPENDIX D: DECAY OF COHERENCES

In this Appendix we keep a single index  $w = (l, s, v)$ , and denote  $w \pm 2 = (l \pm 2, s \pm 1, v)$ . In order to prove that the cumulative coherences decay to zero on the slow time scale, we rewrite Eq. (56) in the form

$$\dot{r}_{ww'} = \dot{r}_{ww'}^{DB} + \dot{r}_{ww'}^{NEG}, \quad (D1)$$

where the first term

$$\dot{r}_{ww'}^{DB} = 2\Gamma_{\downarrow}^{(1)}[f_{w+2}f_{w'+2}r_{w+2w'+2} - f_w f_{w'} r_{ww'}] + 2\Gamma_{\uparrow}^{(1)}[f_w f_{w'} r_{w-2w'-2} - f_{w+2} f_{w'+2} r_{ww'}], \quad (D2)$$

corresponds to a set of kinetic equations with (positive) rates that fulfill detailed balance conditions. The matrix that enters the right hand side and generates the evolution is therefore evidently non-positively defined, and has exactly one eigenvector with zero eigenvalue, corresponding to the stationary solution of the Boltzmann-Gibbs form.

The second term in Eq. (D1)

$$\dot{r}_{ww'}^{NEG} = -2\Gamma_{\downarrow}^{(1)} \left[ \frac{1}{2} (f_w^2 + f_{w'}^2 - f_w f_{w'}) r_{ww'} \right] - 2\Gamma_{\uparrow}^{(1)} \left[ \frac{1}{2} (f_{w+2}^2 + f_{w'+2}^2 - f_{w+2} f_{w'+2}) r_{ww'} \right], \quad (\text{D3})$$

corresponds to a set of simple decay equations, with the rates which are evidently positive, since  $\frac{1}{2}(f_w^2 + f_{w'}^2) - f_w f_{w'}$  is strictly greater than zero for  $w \neq w'$ .

The full dynamics of the cumulative coherences is thus generated by the sum of the two matrices, one of which is non-positively defined, and the other being strictly negatively defined. The sum itself must therefore be negatively defined, *ergo* it generates the decay to zero.

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